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Experimental observation of phonons as spectators in FeSi electronic gap formation

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The evolution of a phonon spectrum in a narrow-gap semiconductor FeSi was investigated in a wide range of temperatures (46 K $\leqslant T \leqslant$ 297 K, $P = 0.1$ MPa) and pressures (0.1 MPa $\leqslant P \leqslant$ 43 GPa, $T = 297$ K) using nuclear inelastic scattering of synchrotron radiation with the energy resolution 0.53 meV. Decreasing temperature as well as increasing pressure causes a strong reorganization of the phonon spectrum manifested in splitting and shifts of the phonon peaks. The phonon spectra measured under the temperature and pressure conditions corresponding to the same unit cell volume reveal nearly complete matching. On the contrary, the spectra measured under the conditions of the equal mean-square atomic displacements differ drastically. These observations suggest that the transformation of the electronic spectrum of FeSi is controlled predominantly by the change of the unit cell volume. The corresponding changes of the interatomic forces and the resulting modification of the phonon spectrum appear as the direct consequence of this transformation.

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The intensively studied and permanently expanded class of the compounds termed as strongly correlated electron systems (SCES) is characterized by an essential interaction between conduction electrons and localized electrons of partially filled f (or d) shells [1]. Tiny nuances of this interaction provide the conditions responsible for the formation of all the unusual properties of SCES. At low temperatures these systems can appear, for example, as semiconductors with a narrow gap between a valence and a conduction band, which is generally believed to be the result of hybridization effects. The strong rearrangement of an electronic spectrum near the Fermi energy occurs with a temperature increase: The gap in the electron density of states is closed, and the Kondo-metal behavior takes place [2]. The main question related to these systems is the origin of driving forces for this insulator-to-metal transition.

Conduction electrons provide a considerable influence on the formation of the spectrum of atomic vibrations in metals. This influence is manifested, for example, in a number of experimentally observed effects: (i) softening of a phonon spectrum due to conduction electron screening of the interatomic potentials [3]; (ii) an occurrence of singularities in a group velocity of phonons for specific wave vectors [4,5]; (iii) an influence of the opening of the gap in an electronic spectrum on a phonon lifetime [6], etc. The examples of the interaction of the electronic subsystem with the selected phonon modes were recently observed even for the strongly correlated systems as high-temperature superconductors [7] and Kondo insulators [8], not related to the classical case of the mixed valence compounds [9].

The opposite examples of the influence of the phonon subsystem on the electronic subsystem are known as well. For instance, for V_3Si and V_3Ge systems with $A15$ structure, the disorder caused by atomic thermal vibrations at temperatures above the Debye temperature leads to a decrease of an electronic density of states at the Fermi level [10]. This effect, in turn, decreases screening activity of conduction electrons that is manifested in the abnormal increase of phonon energies with increase of temperature. Thus, for $A15$-type substances, the atomic thermal vibrations (phonons) indeed affect the electronic subsystem, and its transformation leads to hardening of the phonon frequencies. For SCES, however, an interaction and interplay of electronic and phonon subsystems is not yet understood and requires experimental studies.

Iron monosilicide FeSi is a particular example of SCES with d-electrons, which has attracted much attention because of its unusual noncentrosymmetric crystal structure and anomalous temperature dependencies of magnetic, optic, elastic, and transport properties [11–16]. At low temperatures, FeSi behaves as a narrow-gap semiconductor with the gap of about 30 meV near the Fermi level. With increasing temperature the gap becomes closed, and at $T \sim 150$ K a transformation to a metallic phase is developed [13,16]. Infrared spectroscopy reveals that with increasing temperature the width of the gap decreases, i.e., the gap collapses [17]. Photoelectron spectroscopy shows that the gap is filled from the bottom and completely disappears [16] at $T = 200\,K$. The driving mechanism for this transition so far is not clear.

The reorganization of the electronic spectrum related to the closure of the gap in the density of electron states affects the interatomic interaction in FeSi and, therefore, changes the spectrum of the lattice excitations. This, for example, was

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demonstrated in Refs. [18,19] in observations of a pronounced softening of the phonon spectrum with temperature. In both studies, the effect observed in phonon properties is attributed to closing the gap in the electronic spectrum.

However, the reason for the underlying closing of the electronic gap with temperature is not yet clear. In Ref. [18], the closing of the gap is attributed to the effect of thermal disorder [20], i.e., to the influence of enhanced thermal vibrations on the electronic structure. Within this scenario, the influence of the phonon system on the electronic system appears as a driving force of the transformation of FeSi properties with temperature.

However, it is well known that significant rearrangements of an electronic spectrum can also be caused by even a small change of the unit cell volume. Therefore, the closing of the gap in the electronic spectrum of FeSi with temperature can, in general, be caused by an increase of the unit cell volume due to a thermal expansion. Thus, the measurements of only the temperature dependence of the phonon spectrum are not conclusive to distinguish which of the two factors—the change of the atomic vibrations amplitude or the change of the unit cell size—has the dominating impact to the modification of the electronic spectrum.

A more appropriate approach would be to study both temperature and pressure dependencies. Temperature and pressure influence differently the amplitude of atomic vibrations and the unit cell volume. This should allow for understanding which of the subsystems—phonon or electronic one—plays the role of a "actor" and which one remains a "spectator".

In terms of the sensitivity of the lattice vibrations to the transformation of the electron spectra in the gap energy region, the most optimal way seems to be to study the dynamics of iron atoms. Indeed, the electronic spectrum of FeSi near the Fermi level is formed mainly by *d*-electron states of iron [21]. Therefore, the rearrangement of the electronic spectrum due to the closing the gap and the corresponding release of free-charge carriers affects first of all the bonding forces of iron atoms and should be reflected in the iron partial phonon density of states (PDOS). Therefore, the study of the correlations between the iron partial phonon spectrum and the electron subsystem under variable external parameters can provide important information about physics of the metal-insulator transition in SCES as FeSi.

In this work, we studied the dynamics of iron atoms in FeSi by nuclear inelastic scattering of synchrotron radiation [22–25] and derived the iron partial PDOS with very high energy resolution. The studies were performed as a function of two external parameters: temperature and pressure. Temperature affects mainly the amplitude of the atomic vibration, whereas pressure influences mostly the unit cell volume. Therefore, the analysis of the temperature and pressure effects allows for an empirical, i.e., model-independent, evaluation of the relative roles played by the amplitude of atomic vibrations and by the size of the unit cell.

The sample of iron monosilicide FeSi was synthesized by inductive melting from a 1:1 mixture of high-purity silicon and iron enriched in the ^{57}Fe isotope up to 94.5%. X-ray powder diffraction confirmed a single-phase state of the sample with the structure of cubic FeSi (spatial group $P2_13$). The lattice constant of the crystal determined at room temperature is $a = 4.486 \pm 0.001$ Å, which agrees with the published data [11,26].

For temperature studies, the sample with the mass of 7 mg was attached to the cold finger of a closed-cycle helium cryostat. For pressure studies, the sample with the mass of 0.6 μg was placed in the diamond anvil cell with a paraffin as the pressure-transferring medium. The pressure values were determined from the shift of the luminescence line of the ruby chip located near the sample both before and after the measurements of nuclear inelastic scattering. The quoted values of pressure and their error bars were determined from the mean value and the difference of the two pressure measurements, respectively.

The energy dependencies on nuclear inelastic scattering were measured at the Nuclear Resonance beamline ID18 [27] of the European Synchrotron Radiation Facility. The measurements were performed in the energy range from -10 meV to $+90$ meV around the energy of the nuclear resonance transition of the ^{57}Fe isotope (14.4125 keV) with the energy resolution of 0.53 meV (full width at half maximum, permanent within the studied range of the energy transfer). The storage ring was operated in a $7/8 + 1$ mode. For this mode, sufficient statistical accuracy was achieved after ~20 h of measurements by adding ~35 scans. The temperature set of data was taken at 46, 103, 153, 180, 205, 251, and 297 K at ambient pressure. The pressure data set was taken at ambient pressure, at 0.49(6), 0.96(8), 2.0(1), 11.9(5), 21.0(9), and 43(2) GPa at room temperature.

The iron partial PDOS was derived from the obtained experimental spectra using the standard double Fourier transform procedure [28], which includes a proper subtraction of the multiphonon contributions. Data processing was carried out in a quasiharmonic approximation, which is justified for the investigated ranges of temperature and pressure. The area under the derived PDOS curve is equal to unity. Further details of the experimental setup, technique, and data processing can be found elsewhere [28,29].

The obtained temperature and pressure dependencies of the iron partial PDOS of FeSi are shown in Figs. 1(a) and 1(b), respectively. The high-energy resolution utilized in present studies for the first time allowed for the observation of the fine structure of the PDOS, which was not visible in earlier works [18,30]. In particular, Fig. 1 shows that the effect of opening the gap in the electronic spectrum of FeSi on its phonon system is not limited only to phonon hardening. In fact, the broad maximum observed by neutron scattering [18] at 22–28 meV consists of three peaks. Two of them are well resolved at all temperatures. In addition, the lower-energy maximum demonstrates the enhancement of splitting into two peaks with a decrease of temperature [Fig. 1(a)]. A very similar picture is observed for pressure dependence: two peaks stay well resolved for all pressures, and an additional splitting of the lower-energy peak develops with an increase of pressure [Fig. 1(b)].

The opening of the gap in the electronic structure of FeSi should be accompanied by an inhomogeneous readjustment of the energies of various phonons. This readjustment is apparently revealed in the rearrangement of the low-energy part of the iron partial PDOS by the development of the splitting for the dominant group of the peaks around of 24 meV (Fig. 2).

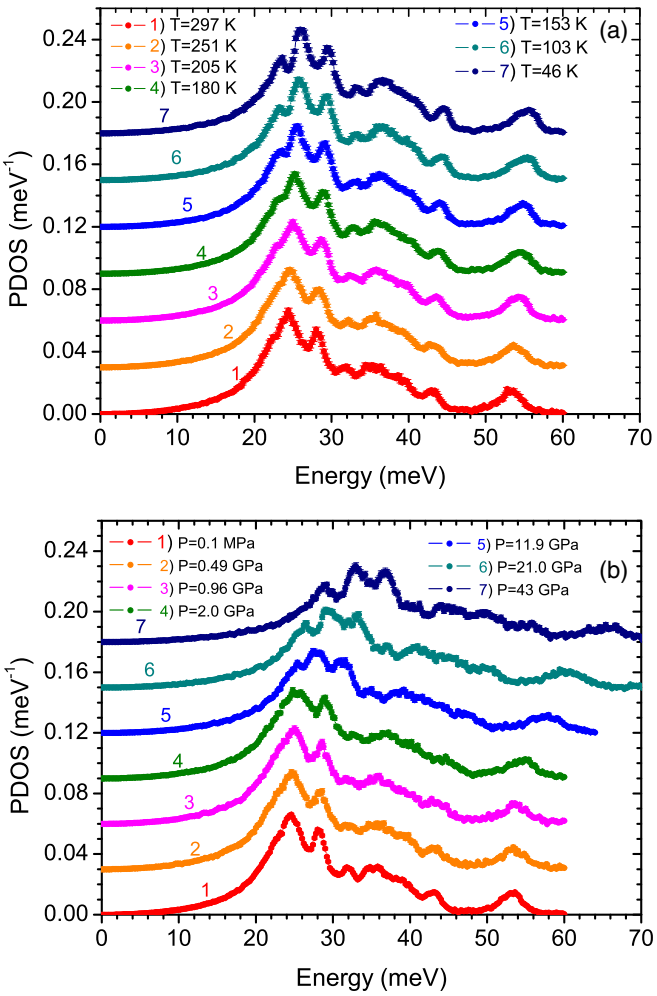

FIG. 1. The evolution of the partial DOS of iron atoms in FeSi: (a) with temperature at ambient pressure; (b) with pressure at room temperature. For easier visibility, the curves are shifted vertically.

Indeed, according to the model calculations of the lattice dynamics for monosilicides of iron group, these peaks should be related to the contribution to the phonon spectrum from the longitudinal acoustic vibrations with the wave vectors at the Brillouin zone boundary and from the low-energy weakly dispersive optical modes [18,31]. These modes are associated mainly with the vibrations of iron atoms, the energies of these modes are in the range of the estimated energy of the gap in the electronic spectrum, and these phonons are most sensitive to the change of the electron-phonon interaction [19,32]. The observed splitting of the first maximum in the phonon spectrum is obviously caused by the change of the dispersion for some of these modes. Therefore, it is apparently related to the modification of the interatomic interaction caused by the opening of the gap in the electronic spectrum on decreasing temperature or increasing pressure.

The above theoretical considerations are confirmed by experimental data. For instance, the steplike increase of the width of the first peak in the PDOS of FeSi with temperature observed in Ref. [19] occurs at the critical temperature $T_c =$ 180 K which corresponds to the temperature of the metal-semiconductor transition. Furthermore, the similar steplike

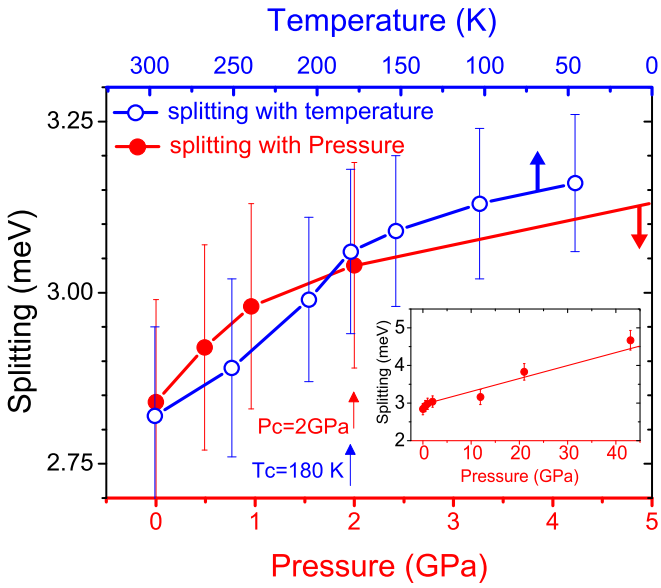

FIG. 2. The temperature and pressure dependences of the splitting for the two lowest-energy peaks in the PDOS, displayed by the open and filled symbols respectively. The vertical arrows labeled by T_c and P_c indicate the critical temperature and pressure of the metal-semiconductor transition, respectively. Inset: The pressure dependence of the splitting for the two lowest-energy peaks in the PDOS for all range of investigated pressures.

broadening of the optical phonon mode with the energy of 22.3 meV was observed at nearly the same temperature by Raman spectroscopy [32]. The broadening occurs only for the semiconducting (not for metallic) samples, and its evolution with temperature corresponds to the activation energy of 30 meV, which matches precisely the gap value in the electronic spectrum [32]. Thus, the transformation of the phonon dynamics at the energies of about 24 meV is indeed tightly related to the opening of the gap in the electronic system at the critical temperature of $T_c \sim 180$ K.

Figure 1 demonstrates that the development of the splitting for the peaks around 24 meV with increasing pressure [Fig. 1(b)] is very similar to that with decreasing temperature [Fig. 1(a)]. Since the temperature evolution of the PDOS is attributed to the opening of the gap, the similar pressure evolution also should be caused by the rearrangement of the electronic structure and opening of the gap at increasing pressure.

In order to estimate the evolution of the various parts of the PDOS quantitatively, each of the spectra measured at various temperatures and pressures was fit by a set of eight Lorentzians according to the number of the peaks observed in the energy range above 20 meV. The temperature and pressure evolutions of the splitting for the two lowest-energy peaks are shown in Fig. 2. For the critical temperature $T_c = 180$ K of the metal-semiconductor transition, the splitting of the first two (yet not completely resolved) peaks is 3.06(0.12) meV. In pressure dependence, almost the same splitting 3.04(0.15) meV is observed at $P = 2.0$ GPa. This confirms that the critical pressure $P_c = 2$ GPa indeed corresponds to a transition of FeSi to the semiconducting state at room temperature. As will be shown below, the transitions at 180 K (ambient pressure) and

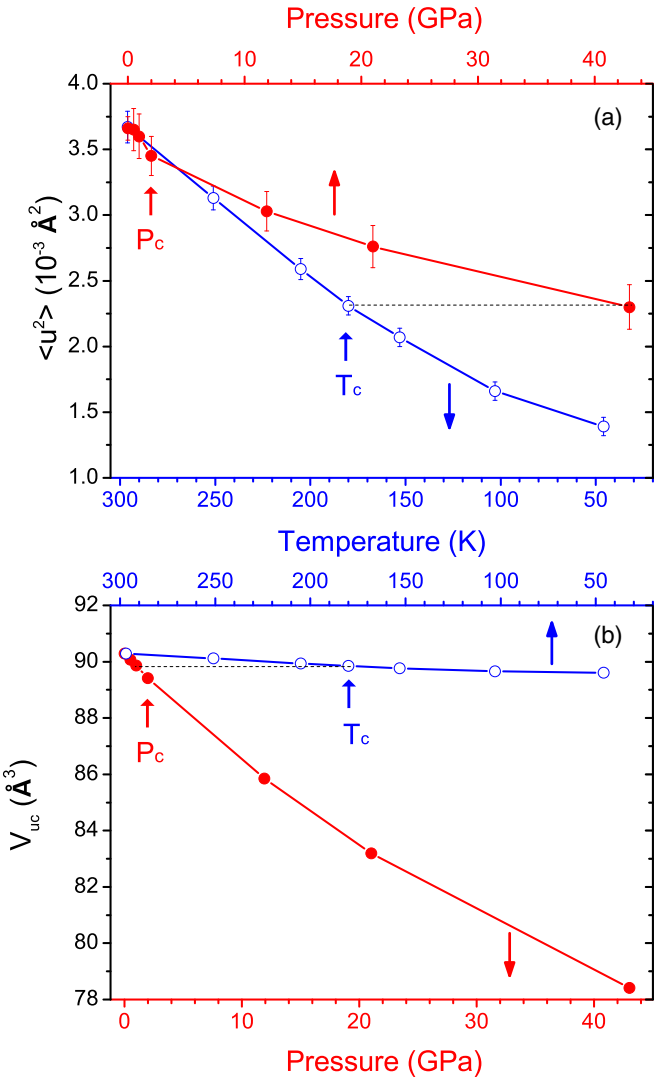

FIG. 3. The temperature and pressure dependences (a) of the mean-square amplitude $\langle u^2 \rangle$ of atomic vibrations and (b) of the unit cell volume V. T_c and P_c indicate the temperature and pressure of the onset of the splitting of the first phonon peak, respectively. The dashed horizontal lines show the mean-square amplitude (a) and unit cell volume (b) at $T = T_c$.

2 GPa (room temperature) occur at nearly the same volumes of unit cell but notably different amplitudes of atomic vibrations.

The temperature and pressure dependencies of the mean-square amplitude $\langle u^2 \rangle$ of atomic vibrations and the unit cell volume V are shown in Figs. 3(a) and 3(b), respectively. The mean-square amplitudes of atomic vibrations for various temperatures and pressures were obtained directly from the raw spectra of nuclear inelastic scattering and cross-checked by the alternative calculations from the derived PDOS [29]. The quoted uncertainty of the reported values of $\langle u^2 \rangle$ was evaluated from the difference between the above two values. The temperature dependence of the unit cell volume was calculated from the thermal expansion coefficient of FeSi reported in Ref. [26] and the unit cell volume at room temperature (297 K) $V_0 = 90.28 \pm 0.06$ Å^3 measured in this work. The pressure dependence of the unit cell volume was calculated using the third-order Birch-Murnaghen [33] equation of state reported in Ref. [34] using $V_0 = 90.28 \pm 0.06$ Å^3. The uncertainties of the derived mean-square amplitudes are determined by the statistical accuracy of the measured spectra of nuclear inelastic scattering. The uncertainty of the derived unit cell volume is dominated by the error bar of the unit cell volume measured at ambient conditions, except for the last three pressure points, where it is determined by the error bars of the pressure measurements evaluated as described above.

Figure 3 shows that the volume of the unit cell and the mean-square amplitude of atomic vibrations change very differently with temperature and pressure. The amplitude of atomic vibrations strongly depends on temperature and weaker on pressure [Fig. 3(a)]. On the contrary, the unit cell volume is only slightly affected by temperature but strongly changes with pressure [Fig. 3(b)].

If the dominating factor in the opening of the electronic gap is thermal disorder, then the enhancement of the splitting of the first maximum of the PDOS for temperature and pressure measurements should occur at the same (or close) values of the amplitude of atomic vibrations. For temperature measurements, the enhancement of the splitting observed at the critical temperature $T_c = 180$ K corresponds to the mean-square amplitude $\langle u^2 \rangle = 2.31 \times 10^{-3}$ Å^2 [Fig. 3(a)]. For pressure measurements, this value of the mean-square amplitude is reached only at the highest pressure of 43 GPa [Fig. 3(a)]. On the contrary, the enhancement of the splitting at the critical pressure $P_c = 2$ GPa corresponds to the much larger mean-square amplitude $\langle u^2 \rangle = 3.46 \times 10^{-3}$ Å^2 [Fig. 3(a)]. Thus, thermal disorder apparently is not the reason for the opening of the gap in the electronic structure and the corresponding rearrangement of the PDOS.

Alternatively, if the decisive factor in the opening of the gap is the size of the unit cell, then the enhancement of splitting for temperature and pressure measurements can be expected at the same (or close) unit cell volumes. For temperature measurements, the critical temperature $T_c = 180$ K corresponds to the unit cell volume $V = 89.85$ Å^3 [Fig. 3(b)]. For pressure measurements, the similar unit volume ($V = 89.86$ Å^3) is reached at 0.96 GPa [Fig. 3(b)]. This "equal-volume" pressure is only slightly lower than the critical pressure $P_c = 2$ GPa but much closer to this value than the considered above the equal-amplitude pressure of $P = 43$ GPa. This strongly suggests that the size of the unit cell is indeed the dominant reason for the opening of the gap in the electronic structure and the corresponding rearrangement of the PDOS. The slight mismatch between the critical pressure $P_c = 2$ GPa and the estimated equal-volume pressure of $P_c' = 0.96$ GPa can possibly be attributed to an additional temperature factor: At higher temperature, the same concentration of the free-charge carriers is populated at the slightly larger electronic gap and, accordingly, at somewhat higher pressure.

The dominant role of the unit cell volume in the opening of the gap in the electronic structure and the corresponding reformation of the phonon spectrum can also be seen directly from the comparison of the PDOS measured at (i) equal unit cell volumes and (ii) equal mean-square amplitudes of atomic vibrations. Figure 4(a) compares the PDOSs measured at $T = 180$ K (ambient pressure) and $P = 0.96$ GPa (room temperature). This corresponds to the essentially different

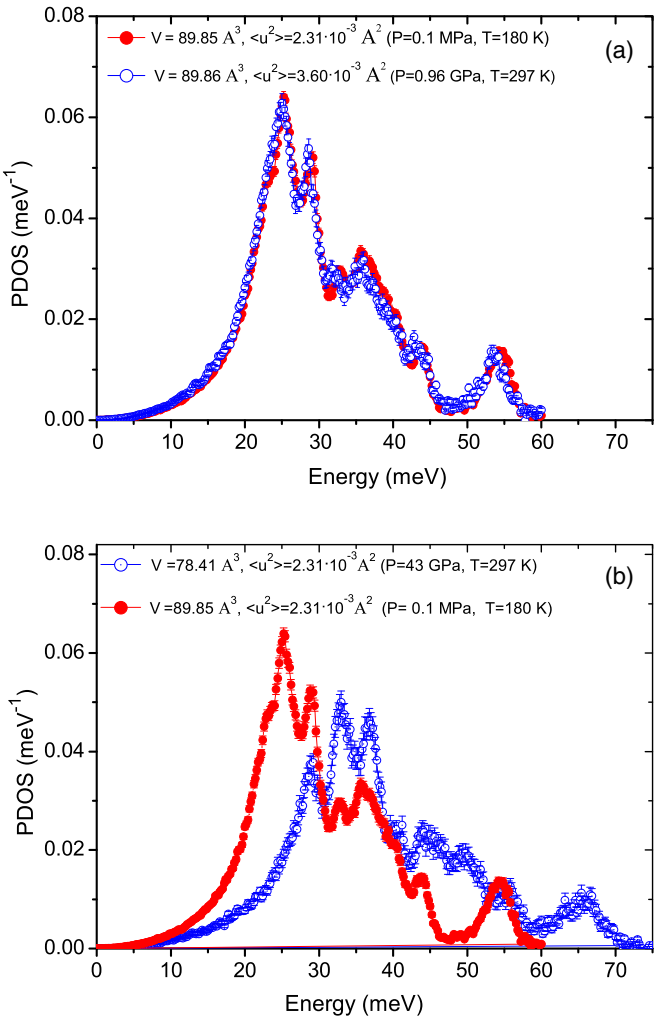

FIG. 4. The partial DOS for iron atoms in FeSi measured (a) for the same unit cell volume V but different mean-square amplitudes $\langle u^2 \rangle$ of atomic vibrations and (b) for the same mean-square amplitudes but different unit cell volumes.

mean-square amplitudes of atomic vibrations (2.31×10^{-3} Å^2 and 3.60×10^{-3} Å^2, respectively), but to nearly the same volume of the unit cell (89.85 Å^3 and 89.86 Å^3, respectively). The PDOS measured at the equal unit cell volumes but different vibration amplitudes are practically identical [Fig. 4(a)]. Figure 4(b) compares the PDOSs measured at $T = 180$ K (ambient pressure) and $P = 43$ GPa (room temperature). This corresponds to the same amplitude of atomic vibrations (2.31×10^{-3} Å^2), but different volumes of the unit cell (89.85 Å^3 and 78.41 Å^3, respectively). The PDOS measured at equal vibration amplitudes but different unit cell volumes are strongly different [Fig. 4(b)]. Thus, the opening of the gap in the electronic structure of FeSi and the corresponding transformation of the phonon spectrum appears to be controlled mainly by the size of the unit cell, and it is not at all sensitive to thermal disorder.

The experimental data obtained in this work do not confirm the suggested earlier correlations of the considerable reorganization of the phonon spectra with the change of the amplitude of atomic vibrations and, most probably, rule out the effect of the thermal disorder as the driving force for the insulator to metal transition and related features in the atomic dynamics of FeSi. In more general terms, the presented results shows that while the influence of the phonon system on the electronic structure may be expected [20], this does not occur for FeSi, where the role of a "actor" belongs to the electron system, whereas the phonon systems remains a "spectator".

Finally, we note that up to now the experimental studies of the lattice dynamics in relation to the opening of the semiconducting or superconducting energy gap at the Fermi energy were performed only with a limited number of SCES. For a few of these systems quite interesting specific features have been observed related, however, not to the energy rearrangement of the phonon spectra but mainly to the modifications of particular phonons' intensity [7,8]. In this content, FeSi is the first example of the strong energy rearrangement of phonons in relation to the electronic gap formation, expected from general consideration of electron-phonon coupling [3].

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